

Superheavy magic structures and relativistic pseudo-spin symmetry

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We have explored the occurrence of the spherical shell closures for superheavy nuclei in the framework of the relativistic Hartree-Fock-Bogoliubov (RHFB) theory and the shell effects in terms of two-nucleon gaps $\delta_{2n(p)}$. Although the results depend slightly on the forces used, the general set of magic numbers beyond ^{208}Pb are predicted as $Z = 120, 138$ for protons and $N = 172, 184, 228$ and 258 for neutrons, respectively. Specifically the RHFB calculations favor the nuclide $^{304}120$ as the next spherical doubly magic one beyond ^{208}Pb . As indicated by the self-consistent calculations, the occurrences of superheavy shell closures are essentially related with the violation and restoration of relativistic pseudo-spin symmetry. Further analysis imply that the shell effects are sensitive to both the values of scalar and nonrelativistic effective masses, which together with the violation of the relativistic symmetry may interpret the origin of model deviations.

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For a fairly long period, it remains a challenging issue in nuclear physics to explore the mass and charge limit of realistic nuclei, i.e., the superheavy elements (SHEs) with $Z \geq 104$ and the so-called stability island of superheavy nuclei (SHN). Far from being simply large clusters of nucleons, these fascinating species owe their very existence to subtle contributions to the nuclear binding energy [1]. The theoretical studies, including the macroscopic-microscopic models [2, 3] and self-consistent mean field approaches [4, 5], have provided a large amount of valuable information for the exploration of SHN. Many efforts have been devoted to finding the next stability island, i.e., the magic SHN with the enhanced stability promised by the shell effects. Although the consensus is somehow reached on the spherical neutron shell closure $N = 184$, other possible neutron magic shells such as $N = 172$ and the next spherical proton shell probably lying in the range of $114 \leq Z \leq 126$ are still being under discussions [6, 7].

Experimentally, the discoveries of new elements up to $Z = 118$ have been reported in Refs. [8, 9]. However, these SHN are not located on the stability island as originally sought. In addition the enlarged survival probabilities with increasing proton number of SHEs from $Z = 114$ to 118 seem to indicate the enhanced shell effects with increasing Z and therefore a possible proton magic shell may emerge beyond $Z = 118$ [10].

On the other hand, the extrapolation towards the superheavy region also challenges the predictive reliability of nuclear structure models. The macroscopic-microscopic methods, although generally successful in describing the nuclear binding, require preconceived knowledge of the expected densities and single-particle (s.p.) potentials [2], which fades away when stepping into new regions where stronger polarization effects and more complicated functional forms of the densities may occur [4]. It is well known that the SHN are mainly stabilized by the shell effects, and the self-consistency of the theory is therefore of special significance for a reliable description of SHN. In fact, the shell effects are essentially related with the nuclear spin-orbit(SO) splittings and relevant pseudo-spin symmetry restoration [11] as well as the shape of the nucleus. Whereas the variations of SO splitting are mainly

determined by both SO potential concerned with the derivative of the average potential and the tensor force originated from the exchange of pion [12]. This leads to a challenging and ambitious task to provide a unified self-consistent description of both spin-orbit coupling and tensor effects, which can be achieved on the level of the relativistic Hartree-Fock (RHF) approach under the meson exchange picture of nuclear forces.

In the past years, the covariant density functional (CDF) theories [13, 14] have achieved great success in the self-consistent description of nuclear systems, including the stable and weakly bound nuclei and neutron stars. One of existing approaches is the density-dependent relativistic Hartree-Fock (DDRHF) theory [15, 16] and its extension — the relativistic Hartree-Fock-Bogoliubov (RHFB) theory [17]. Within DDRHF, the Lorentz covariant structure is fully kept, thus ensuring the natural treatment of nuclear spin-orbit couplings. The inclusion of Fock terms in DDRHF not only brings substantial improvements in self-consistent descriptions of nuclear structure properties [18–20] and neutron star physics [21, 22], but also provides the natural origin of the nuclear tensor force, e.g., the pion exchange and ρ -tensor couplings [16, 18].

As an important residual interaction beyond the p-h channel, the pairing correlations not only contribute to the stability of SHN but also play a major role in determining the nuclear deformation [23], which requires a unified self-consistent description of the mean field, pairing field and nuclear deformation. In terms of Bogoliubov quasi-particles, such a goal is partially achieved by the RHFB theory which unifies the description of RHF mean field and pairing correlations. Although a complete RHFB study would require to explore also the shape degrees of freedom [24] — a very time-consuming task — one can already discuss the spherical magicity of SHN in the spherical RHFB calculations.

In this work we investigate the superheavy nuclides covering $Z = 110 \sim 140$. In the pairing channel, the finite-range Gogny force D1S [25] renormalized by a strength factor f is adopted as effective pairing interaction. The introduction of the factor f is due to the fact that the pairing related quantities, such as the odd-even mass differences and the moments of inertia, are systematically overestimated in the RHFB calcula-

tions of heavy nuclei with the original Gogny pairing force [26]. To eliminate such systematical deviations, the strength factor is reduced as $f = 0.9$ by reproducing the odd-even mass differences of odd Pb isotopes. Concerning the RHF mean field, the adopted effective Lagrangians are PKA1 [16] and PKO series [15, 18]. For comparison the relativistic Hartree-Bogoliubov (RHB) calculations [14] with PKDD [27] and DD-ME2 [28] are also presented in this work. The integro-differential RHF equations are solved on a Dirac Woods-Saxon basis [29] with a radial cutoff $R = 28$ fm. The numbers of positive and negative energy states in the basis expansion for each s.p. angular momentum (l, j) are chosen to be 44 and 12, respectively.

To identify the magic shells, different observables can be chosen, such as nucleon separation energies, pairing gap energy, s.p. spectra, etc. The magic shells in SHN might not be as well-marked as in the ordinary nuclei. Here, we concentrate on two types of observables. One is the so-called two-nucleon gaps [δ_{2p} (proton) and δ_{2n} (neutron)], i.e., the difference of two-nucleon separation energies of neighboring isotopes or isotones, which provides an efficient evaluation of the shell effects,

$$\delta_{2p}(N, Z) = S_{2p}(N, Z) - S_{2p}(N, Z + 2), \quad (1a)$$

$$\delta_{2n}(N, Z) = S_{2n}(N, Z) - S_{2n}(N + 2, Z). \quad (1b)$$

Obviously, the peak values of the two-nucleon gaps are essentially determined by the sudden jump of the two-nucleon separation energies, which can be taken as the evidence of the magic shell occurrence.

Fig. 1 presents the two-proton (left panels) and two-neutron (right panels) gaps for the even-even isotopes of $Z = 110 \sim 140$, calculated with the selected effective Lagrangians. The thick stepped lines show the two-proton drip lines identified by two-proton separation energies. Nuclei that are stable with respect to β -decay and fission in our calculations are emphasized by filled stars and circles, respectively. The β (or fission)-stability line is defined by the maximum binding energy per nucleon for a given A (or Z), which corresponds to the minimum Q -value of β -decay (or fission) [31]. The dashed lines denote the empirical β -stability lines described by the formula $Z = A/(1.98 + 0.0155A^{2/3})$ [30]. The open thick squares lying at the lower-left corner of each plot represent the even-even SHN observed or declared to be observed experimentally. It is clearly seen that the experimentally discovered elements coincide remarkably well with the predicted fission stability line, especially for PKA1, although the deformation may play a significant role in stabilizing the SHN. Strictly speaking, only nuclei having negative chemical potentials are stable against nucleon emission. However, due to the strongly enhanced Coulomb barriers in SHN the two-proton drip lines extend by a few more units to the proton-rich side beyond negative chemical potentials. In Fig.1, the squares filled with thicker color stand for the larger gaps and obviously the peak areas indicate the emergence of magic shells.

From Fig. 1 one can see that PKA1 presents the most distinct shell effects, supporting $Z = 120, 126, 138$ and $N = 184, 258$ as the candidates of proton and neutron magic numbers, respectively. The other effective Lagrangians also present

a fairly remarkable proton shell at $Z = 120$. In addition, $Z = 132$ by PKDD and $Z = 138$ by both RHFB and RCHB calculations are found to be possible proton magic numbers, consistent with the predictions in Ref. [5]. Concerning the neutron shells, besides $N = 184$ and 258, PKA1 also presents fairly distinct shell structures at $N = 172$, which is illustrated evidently by the other Lagrangians. Fairly distinct shell effects at $N = 184$ and 258 are also found with the other parametrizations except with PKO2. Remarkable shell effects are also found at $N = 228$, although not so strongly as at $N = 184$ and 258 by PKA1. Furthermore, the occurrence of neutron shells at $N = 164$ is illustrated by PKO2, PKDD and DD-ME2, and the latter two demonstrate another occurrence at $N = 198$.

Inspecting another observable — the pairing gap energies whose zero values accompany the emergence of magic shells, one can achieve similar conclusions as above on the emergence of proton and neutron shells. Combined with the two-nucleon gaps, it is found that the proton shell $Z = 120$ is supported evidently by PKA1, and by the other interactions to some extent. Hence $Z = 120$ can be considered as model-independent candidate of proton magic numbers. On the other hand, the situation for the neutrons is more complex. Although $N = 172$ and 228 seem to be generally supported by the selected effective Lagrangians, the corresponding shell effects are not strong enough to determine the occurrence of magic shells. Except for PKO2, $N = 184$ and 258 are also generally favored as the candidates of neutron magic numbers. Specifically, PKA1 can provide a better description on the nuclear shell structure than the others [16] and better agreement on the fission stability of discovered SHN (see Fig. 1), and presents pronounced shell effects there. In fact, as indicated by Skyrme Hartree-Fock (SHF) investigations [32] $N = 184$ is also favored evidently to be a spherical neutron magic number and the $N = 184$ isotones are expected to have spherical shapes.

TABLE I: Bulk properties of symmetric nuclear matter calculated with the effective interactions PKA1, PKO series, PKDD and DD-ME2: saturation density ρ_0 (fm^{-3}), binding energy per particle E_B/A (MeV), incompressibility K (MeV), asymmetry energy coefficient J (MeV), scalar mass M_S^* and non-relativistic effective mass M_{NR}^* [15] in units of nucleon mass M .

Force	ρ_0	E_B/A	K	J	M_S^*	M_{NR}^*
PKA1	0.160	-15.83	229.96	36.02	0.547	0.681
PKO1	0.152	-16.00	250.24	34.37	0.590	0.746
PKO2	0.151	-16.03	249.60	32.49	0.603	0.764
PKO3	0.153	-16.04	262.47	32.98	0.586	0.742
PKDD	0.150	-16.27	262.19	36.79	0.571	0.651
DD-ME2	0.152	-16.11	250.30	32.27	0.572	0.652

Nevertheless, from Fig. 1 one can find distinct deviations among the models in predicting the magic numbers. $Z = 120$ can be considered as a reliable prediction of proton magic number and $Z = 138$ could be another candidate with more model dependence. The neutron shells $N = 172, 184, 228$ and 258 are common to several models. Other shells, e.g., $N = 198$, appear essentially model dependent. Among the present models, one may notice that RHB calcula-

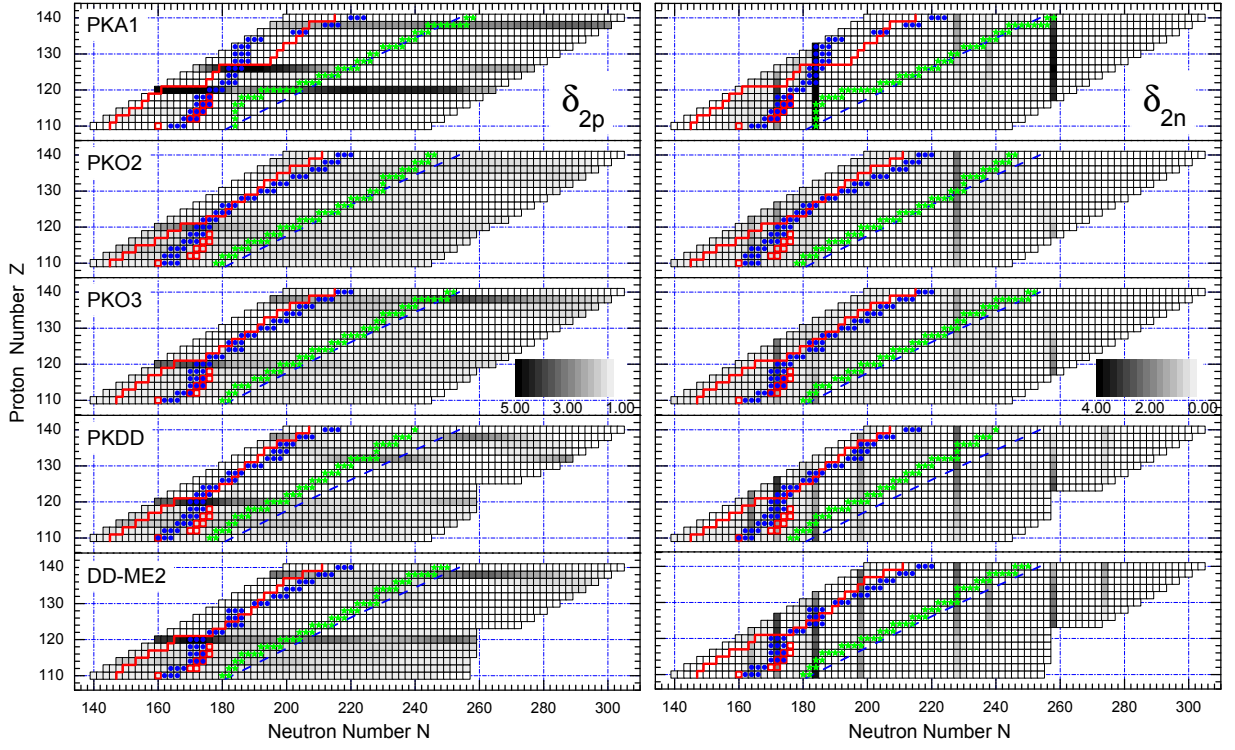


FIG. 1: (Color online) Contour plots (in MeV) of two-proton gaps δ_{2p} (left panels) and two-neutron gaps δ_{2n} (right panel) as functions of N and Z . The results are extracted from the RHF calculations with PKA1, PKO2 and PKO3, and RHB ones with PKDD and DD-ME2. The thick stepped lines show the two-proton drip lines. The nuclei stable with respect to β -decay and fission are marked with filled stars and circles, respectively. The long-dashed lines represent the β -stability line $Z = A/(1.98 + 0.0155A^{2/3})$ [30]. The open thick squares lying at the lower-left corners denote the superheavy nuclei observed or declared to be observed experimentally.

tions (PKDD and DD-ME2) predict more shell closures than the others while PKO2 predicts fewest candidates. To interpret such distinct deviations, Table I shows the bulk properties of symmetric nuclear matter determined by the present sets of Lagrangians. In general the occurrence of superheavy magic shells is closely related with both the scalar mass M_S^* and effective mass M_{NR}^* [15], which essentially determine the strength of spin-orbit couplings and level densities, respectively. Among the present models, the effective Lagrangian PKO2 predicts the largest values of both masses, which leads to relatively weak spin-orbit couplings and high level density on the average. As a result there remains little space in the spectra for the occurrence of magic shells. On the other hand, the RHB models predict more magic shells due to the relatively small masses. In fact, as seen from Fig. 1, PKO2 also presents weaker shell effects than the others. For PKA1 the situation is different. Although it has a larger effective mass M_{NR}^* than PKDD or DD-ME2, PKA1 gives a smaller scalar mass M_S^* and shows stronger shell effects than the others. Due to these reasons PKA1 does not suffer of the common drawback of the CDF calculations — the so-called artificial shell closures [33] — and it better preserves the relativistic symmetry [16, 20]. From this point of view the deviations between models may also originate from the relativistic symmetry restorations.

Similarly to the situation in the stable region [16], the model

deviations originating from the relativistic pseudo-spin symmetry conservation can also be found in the s.p. spectra of SHN. Taking the doubly magic SHN $^{304}_{120}184$ as an example, Fig. 2 shows the proton (left panel) and neutron (right panel) canonical s.p. spectra provided by selected models. It is found that PKA1 provides the most evident magicity at $Z = 120$ and $N = 184$, respectively, although these shell closures are much weaker than in ordinary nuclei. For the neutron shell $N = 184$, it is essentially determined by the degeneracy of two pseudo-spin partners $\{2h_{11/2}, 1j_{13/2}\}$ and $\{4s_{1/2}, 3d_{3/2}\}$, respectively above and below the shell. For the latter, the pseudo-spin symmetry is well preserved in all the calculations while for the former with high angular momentum the symmetry is only properly restored by PKA1 while seriously violated by the others, leading to the occurrence of the shell closure $N = 198$. In fact, a similar emergence of shell closure can also be found in mid-heavy and heavy regions of the nuclear chart. For instance, the proton shell $Z = 82$ in ^{208}Pb can be also taken as the result of the degeneracies of two pseudo-spin partners $\{2f_{7/2}, 1h_{9/2}\}$ and $\{3s_{1/2}, 2d_{3/2}\}$. In the CDF calculations (except PKA1) there is a clear gap between $2f_{7/2}$ and $1h_{9/2}$, i.e., the artificial shell closure $Z = 92$ [33], which somewhat compresses the magic shell $Z = 82$.

A similar mechanism can also be found in the formation of sub-shell 64 due to the degeneracy of the pseudo-spin partners $\{3s_{1/2}, 2d_{3/2}\}$ and $\{2d_{5/2}, 1g_{7/2}\}$ [16]. In the CDF calculations

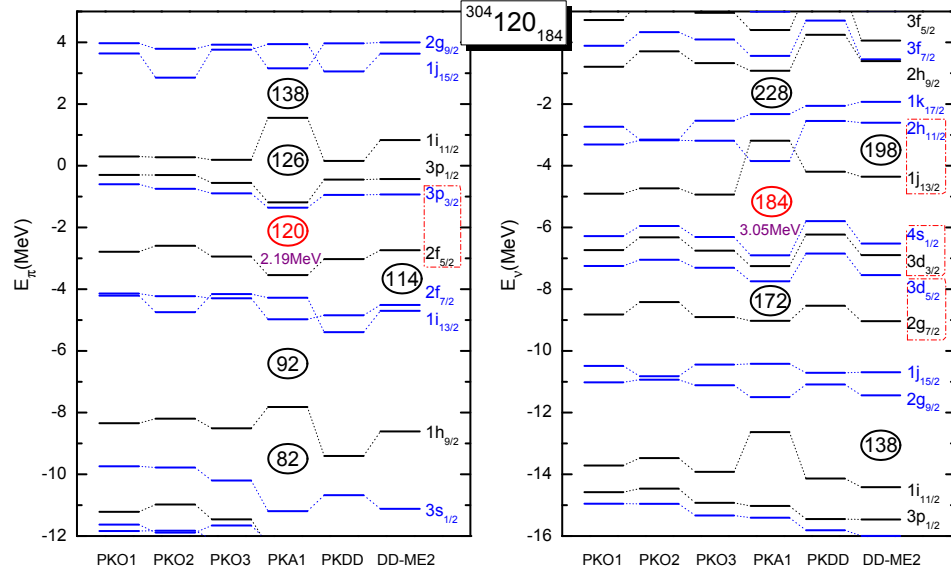


FIG. 2: (Color online) Proton (left panel) and neutron (right panel) canonical s.p. spectra of superheavy nuclide $^{304}_{120}184$. The results are extracted from the RHFB calculations with PKO series and PKA1, as compared to the RHB ones with PKDD and DD-ME2. In all cases the pairing force is taken as the finite range Gogny force D1S with the strength factor $f = 0.9$. See the text for details.

(except with PKA1) the sub-shell 64 is compressed by the violation of pseudo-spin symmetry on the partners $\{2d_{5/2}, 1g_{7/2}\}$, which induces the so-called artificial shell closure 58 [16, 33]. From this point of view, the restoration of pseudo-spin symmetry may also play a delicate role for the occurrence of shell closures in SHN, and this could be another origin of the deviations between the models.

In fact, such tight relation between the relativistic pseudo-spin symmetry restoration and the occurrence of magic shells is not occasionally existing in the superheavy region. It is interesting to notice that there exists at least one pair of pseudo-spin partners above or below the conventional magic shells except $N/Z = 2$ and 8 and the occurrences of shell closures are also favored by the relativistic symmetry restoration to different extent. Traditionally these magicities are interpreted by the strong spin-orbit effects of high- j orbits. While for SHN the increased s.p. levels will 'intrude' the space left by the spin-orbit splitting of high- j orbits such that the restoration of relativistic pseudo-spin symmetry may play more significant roles in determining the occurrence of shell closures. The typical example is the neutron one at $N = 184$ demonstrated by PKA1 (see the right panel of Fig. 2).

Different from $N = 184$, which is favored by the well-preserved pseudo-spin symmetries, the proton shell closure $Z = 120$ emerges with the violation of pseudo-spin symmetry. As shown in the left panel of Fig. 2 the proton shell closure $Z = 120$ is determined directly by the large splittings of two pseudo-spin partner states, $3p_{3/2}$ and $2f_{5/2}$, whereas the spin doublet $3p$ above the shell is nearly degenerated, which can be qualitatively interpreted by the proton configuration. Below the shell $Z = 120$, the protons filling in the high- j states will be driven from the center of nucleus due to the strong centrifugal potential. In addition, the enhanced repulsive Coulomb field in SHN will also expel the protons to spread over large

radial distance. Both effects lead to an interior depression of the proton distributions and consequently the interior region of the mean potential is not flat any more, which may reduce (enlarge) the spin (pseudo-spin) orbital splitting, particularly for low- j states $3p$ and $2f$. In Ref. [34] it is also pointed out that the distinct central depressions on the densities lead to the spherical shell gaps at $Z = 120$ and $N = 172$ as a direct consequence of pseudospin symmetry breaking, whereas a flatter density profile favors the shell occurrence at $N = 184$ as well as the proton one at $Z = 126$. In fact not only for SHN, the emergence of new shell closure $Z/N = 16$ and $N = 32$ [35, 36] can be also related with the violation of pseudo-spin symmetry in light exotic nuclei.

In summary, we have explored the occurrence of spherical shell closures for superheavy nuclei and the physics therein using the relativistic Hartree-Fock-Bogoliubov (RHFB) theory with density-dependent meson-nucleon couplings. The shell effects are quantified in terms of two-nucleon gaps $\delta_{2n(p)}$. To our knowledge, this is the first attempt to perform such extensive calculations within the RHFB scheme. The results indicate that the nuclide $^{304}_{120}184$ could be the next spherically doubly magic nuclide beyond ^{208}Pb . It is also found that the shell effects in SHN are sensitive to the values of both scalar mass and effective mass, which essentially determine the spin-orbit effects and level density, respectively. In addition, the emergence of shell closures is found to be concerned with the violation and restoration of relativistic pseudo-spin symmetry. To some extent, one may further conclude that the model deviations may originate from both effective masses and relativistic symmetry. Experimental measurement of Q_α for at least one isotope of $Z = 120$ nucleus would help us to set proper constraint in determining the shell effects of SHN and further test the reliability of the models as well. One also has to admit that for a more extensive exploration one needs to

take into account the deformation effects.

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